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ADP014625

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SOME CONSEQUENCES OF SOME ASSUMPTIONS WITH RESPECT TO THE PHYSICAL DECAY OF A CHAMBER AEROSOL CLOUD*

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The usual piece of equipment for studying the survival charactersitics of organisms suspended in an atmosphere is a gas-tight chamber controlled with respect to relative humidity and temperature. The mathematical formulation of the behavior of aerosol clouds injected into these chambers and the viability of organisms contained in the particles of these clouds are of great interest to aerobiologists. This paper is concerned with some of the consequences of a particular set of assumptions with respect to the physical decay of chamber aerosol clouds. In presenting the material, I will first touch on those aspects of chambers and aerosol clouds that must be taken into consideration in mathematical formulations. Biological recovery curves will be touched on next. A discussion of relationships among parameters associated with the physical recovery of the cloud will follow -- hitting first the mathematical characterization of the assumptions, then the mathematical relationships among the parameters and finally by means of slides, the relationships will be pointed up visually. The paper will conclude with a short discussion of possible applications of the work and an indication of further work that remains to be done.

Chambers vary enormously in size. Usually they are cylindrical in shape, being oriented either horizontally or vertically. Occasionally they may have a spherical or some other type of shape. The chamber may or may not be revolving. In using a chamber the procedure is to disseminate an aerosol cloud from a liquid slurry containing viable organisms into the chamber.

The aerosol cloud is composed of liquid droplets and the disseminating device produces a spray from the liquid slurry which is similar to the ordinary nose spray used to fight the common cold. Immediately after dissemination, the suspended particles start disappearing from the chamber due to gravitational fallout and impingement on the sides of the chamber. Since

Report on work under Task 2 (Biological Aerosol Decay) or Contract No. DA-18-O64-CML-2810 with the Program Coordination Office at Fort Detrick, Frederick, Maryland.

the larger particles fall more rapidly than the smaller particles, the distribution of particle sizes in the aerosol cloud changes with time. The usual assumption is that the particle number distribution is log normal immediately after dissemination. The fraction of those particles with radii between r and r + dr is f(r) dr where f(r) is the frequency density function of the particle number distribution. Because of the differential fallout of the various sized particles, the particle number distribution does not remain log normal. The usual expression for differential fallout is

$$h(r, t) = \exp(-Kr^2t)$$

where h(r, t) is the fraction of those particles with radii between r and r + dr that remain suspended at time t of those suspended initially. K is a constant that depends on chamber dimensions, gravitational acceleration and other factors. This formula which traces to Stokes law was first derived for stirred stationary chambers by Boyd*. Later Calder** showed that a similar formula held for revolving chambers.

Immediately after dissemination the aerosol particles undergo an equilibration process with respect to their moisture content and the chamber atmosphere. This process ordinarily is accomplished in about a second and so it is convenient to refer to time zero as that instant at which the equilibration process is completed. Both the equilibration and the dissemination process are quite drastic events in the life of an organism and so it is not surprising that many organisms which were viable in the slurry are dead at time zero. The organisms continue to die after time zero. The percentage of those organisms which were viable in the slurry, which remain viable at time zero is known as the initial recovery percentage.

The biological recovery percentage is the ratio, expressed in percentage form, of the number of viable suspended organisms at time t to the number of suspended organisms at time t. In this definition only the

Boyd, Charles A., "The Theory of Sedimentation and Decay of Aerosols", Interim Report BLIR-7, Fort Detrick, July 1952.

^{**}Calder, Kenneth L., 'Some Theoretical Aspects of the Rotating Drum, Aerosol Chamber', BWL Technical Note 13, 1958.

organisms which were viable in the slurry are considered. We will represent the biological recovery percentage as B(t) and thus

Characteristics of the biological recovery curve B(t) as it varies with chamber size and shape, relative humidity, temperature, organism and slurry additives are of great interest to investigators studying the viability of organisms suspended in an atmosphere. The typical biological recovery curve when plotted versus time on semilog paper is concave upward. An estimate of the biological recovery percentage at time t depends on data from a sample of the aerosol cloud withdrawn from the chamber at time t.

There appear to be a number of empirical mathematical expressions that do an excellent job of fitting biological recovery data. These expressions will often explain 99.5 per cent of data variability. The expressions generally have no theoretical basis and give rise to differing consequences. Thus inferences based on these empirical curves are always suspect.

As a step toward deriving biological recovery curves from a more fundamental foundation, BAARINC suggested some time back the heterogeneous initial recovery model. The model postulates that the concave upward curvature of semilog plots is due to nothing more complicated than:

- (1) Distribution of particle sizes,
- (2) Differential fallout of the various sized particles, and
- (3) Higher initial recovery percentages for organisms contained in the larger particles.

These three assumptions are sufficient to generate the type of curvature normally observed. There appears to be no question about the first two postulates. The validity of the third remains to be proven, although it does appear to be quite reasonable to the aerobiologists with whom I have been in contact.

Essentially the heterogeneous initial recovery model states that the biological recovery percentage at time t is a weighted average of the biological recoveries associated with the various sized particles. The weights are the fractions of the suspended organisms that are contained in the various sized particles. These weights continuously change with time. The mathematical formula for the biological recovery percentage at time t is

(1)
$$B(t) = \overline{B}(r, t) = \frac{\int_{O}^{\infty} \sqrt{Nf(r) h(r, t) ar^{s}} B(r, t) dr}{\int_{O}^{\infty} Nf(r) h(r, t) ar^{s} dr}$$

where B(r, t) is the biological recovery percentage for organisms contained in particles with radii between r and r + dr. The number of organisms contained in a particle of radius r is assumed to be proportional to the radius raised to the sth power. Some work by Dr. William C. Day* at Fort Detrick tends to indicate that s may be different from 3.

The weights mentioned a few moments ago are indicated by the trapezoid drawn in the equation above. To point up the logic of these weights, we let N be the number of suspended particles at time zero. Nf(r) dr is then the number of suspended particles with radii between r and r+dr at time zero. Multiplication of Nf(r) dr by h(r, t) yields the number of suspended particles at time t with radii between r and r+dr. Further multiplication by ar^s yields the number of suspended organisms. Hence the denominator of (1) is the number of suspended organisms at time t and the trapezoid ratio is the fraction of suspended organisms contained in particles with radii between r and r+dr.

From equation (1), it is evident that characteristics of the biological recovery curve are intimately tied to the physical aspects of the cloud. In any case an understanding of these physical aspects must precede attempts to ascertain the validity of the heterogeneous initial recovery model.

This work is described by Horner in a Biomathematics Analysis Note. Horner, Theodore W., Fort Detrick, Maryland, Biomathematics Analysis 5082, "A Relationship Between Spore Number and Particle Size", September 14, 1961.

What are reasonable assumptions and what are their consequences. It appears reasonable to assume that f(r) is log normal and h(r, t) is of the form exp $(-Kr^2t)$. Further the mass of a particle, say m(r) is probably proportional to the cube of the particle radius.

To check the validity of these assumptions and to estimate the relevant parameters is not easy for three reasons:

- (1) The particle number distribution does not remain log normal. Part of the present investigation was designed to gain an understanding of the extent of this non-log normality.
- (2) Chambers cannot be sampled at time zero and hence estimates of the parameters of the log normal distribution at time zero must be obtained by indirect means based on data collected after time zero.
- (3) The physical recovery fraction of the cloud involves still another factor; namely, the mass of the particle.

The physical recovery fraction, normalized to 100 per cent recovery at time zero, is given by the formula

(2)
$$R(t) = \frac{\int_{O}^{\infty} Nf(r) h(r, t) br^{3} dr}{\int_{O}^{\infty} Nf(r) br^{3} dr}$$

The mass of a particle is $\overline{m}(r) = br^3$. The total mass suspended at time t and time zero respectively is given by the numerator and denominator of (2).

Following the assumptions made earlier, the recovery fraction is a function of the mean (u), the variance σ^2 of the initial particle number distribution and the chamber constant K. Thus

$$R(t) = R(t; u, \sigma, K).$$

In gaining information about the physical recovery curve one can, on the basis of aerosol samples, do several things. Thus you can:

- (a) Estimate the physical recovery fraction at time t.
- (b) Estimate characteristics of the particle number distribution such as the mean and the variance of Y = ln r. At time zero, y would be a normally distributed variable.

Estimates of $R(t|u, \sigma, K)$, $E(y|u, \sigma, K, t)$ and $Var(y|u, \sigma, K, t)$ can be obtained from the data of aerosol samples, where u and σ are parameters of the log normal distribution at time zero. Knowing these three quantities, it would be desirable to know u, σ , and K. This would provide a basis for checking the validity of the theory concerning K and the log normal, $exp(Kr^2t)$ system in general.

Our work has led to several equations that should be useful in this connection. As mentioned earlier, y was defined as y = ln r. The variables v and q will now be defined as

$$v = (1/\sigma)(y - u)$$

and

(3)
$$q = -(1/2) \ln Kt - u$$
.

Using these definitions, the physical recovery fraction at time t can be written as

$$R(t \mid u, \sigma, K) = R(q, \sigma)$$

where

(4)
$$R(q, \sigma) = (1/\sqrt{2\pi}) \int_{-\infty}^{\infty} \exp \left[-(1/2) v^2 - e^{-2(q-3\sigma^2 - v\sigma)} \right] dv$$

Thus initially, the tabulation of R would have required the four quantities t, u, σ , and K to be taken into account. The q formula relates t, K and u and thus tabulation becomes simpler in that R needs to be computed only as a function of q and σ . One of the slides a little later will show the relationships among R, q, and σ^2 . An approximation formula

has also been developed for computing q as a function of the physical recovery percentage and σ^2 . This formula is useful in generating a starting value of q for iteration procedures for the solution of q given R and σ . The approximation formula is

(5)
$$q = -(1/2) \ln (-\ln R) + \{A + B \ln [-\ln (1 - R)]\} \sigma^2$$

where A and B are appropriate constants.

Using this formula suppose q is calculated given R and σ^2 . If the approximation q is now used to calculate R using equation (5), the calculated R will not differ from the original R by more than O.O2 for the range of σ values pertinent to the present investigation.

Some additional equations are listed below.

(6)
$$\mathbf{E}(\mathbf{y} \mid \mathbf{u}, \ \mathbf{\sigma}, \ \mathbf{K}, \ \mathbf{t}) = \mathbf{u} + \mathbf{\sigma} \mathbf{E}(\mathbf{v} \mid \mathbf{q}, \ \mathbf{\sigma})$$

(7)
$$\operatorname{Var}(y \mid u, \sigma, K, t) = \sigma^2 \operatorname{Var}(v \mid q, \sigma)$$

(8)
$$R(t, u, t, K) = R(q, \sigma)$$

where the frequency density of v is

$$m(v) = \frac{(1/\sqrt{2\pi}) \exp \left[-(1/2) v^2 - e^{-2(q - v\sigma)}\right] dv}{(1/\sqrt{2\pi}) \int_{-\infty}^{\infty} \exp \left[-(1/2) v^2 - e^{-2(q - v\sigma)}\right] dv}$$

Let us look at equations (7) and (8). These are two simultaneous equations. Having estimates of Var y and R(t) available at time t, one can solve for estimates of q and σ . Estimates of q and σ make possible an estimate of $\sigma E(v \mid q, \sigma)$. This latter estimate, when coupled with an estimate of

 $E(y \mid u, \sigma, K, t)$, makes possible an estimate of u. Equation (3) can be solved for the chamber constant K. This constant is a function of q and u. Since estimates of q and u are available, it is now possible to estimate K. Thus from estimates of q and u are available, it is now possible to estimate K. Thus, from estimates of R, E and Var y at time t, one can determine u, σ , and K.

The relationships among these quantities can best be pointed up by means of graphs. For the graphs to be meaningful, it is necessary to make appropriate choices for the parameters u and σ of the log normal distribution of particle sizes at time zero. For u, the range from O.5 to 5μ seems appropriate in the subject matter area to which this investigation is related. Similarly, an upper bound for σ appears to be in the neighborhood of 1.5. To arrive at this latter number we define two radii r_1 and r_2 such that 50 and 84.13 per cent of the particles at time zero have radii less than r_1 and r_2 , respectively. Under these assumptions,

$$\ln r_2 = u + \sigma$$

and

$$ln r_1 = u$$

Hence

$$\sigma = \ln (r_2/r_1)$$

and

$$r_2/r_1 = e^{\sigma}$$

When σ is 1.5, the ratio of the two radii is 4.4817. Thus the radius associated with the 84.13 per cent point is 4.48 times the radius for the 50 per cent point when σ = 1.5. Thus σ = 1.5 appears to be a reasonable upper bound for the subject matter under investigation. In developing tables, the values of σ shown below were used.

<u>σ</u>	r_2/r_1
O.40547	1.0
O. 69315	2. O
1. O 9861	3. O
1. 38629	4. O

Figures 1, 2, 3, and 4 [figures are at the end of this article.] illustrate various parameter relationships. Figure 1 shows the relationships among the physical recovery fraction, q and σ^2 . Each line is associated with a different physical recovery fraction. These lines are almost but not quite straight; the curvature is most pronounced in the lines associated with the lower physical recoveries.

Figure 2 shows the relationships between q, R, and Var y, each line being associated with a different physical recovery fraction. Again these lines are almost straight; the greatest curvature being associated with the lowest physical recovery fractions.

The third figure shows the relationships among (1/Var v), Var y and R. This graph can be used to estimate σ^2 from estimates of R and Var y. The estimate of σ^2 is the product of the estimates of Var y and (1/Var v). Thus suppose R at time t is estimated as 50 per cent and Var y is estimated as 0.43. The value of (1/Var v) is then estimated as 1.12. The estimate of σ^2 is then $(0.43) \times (1.12) = 0.48$.

The final figure shows relationships among (- σ Ev), R and the standard deviation of y. The estimate of u is found by adding (- σ Ev) to the estimate of Ey. Again suppose R = 0.50 and σ_y^2 = 0.43. In this case σ_y = 0.66 and the estimate of (- σ Ev) is 0.065 μ . Thus the estimate of u is found by adding 0.065 to the estimate of u.

Hopefully, the relationships which have been developed will lead to

- (1) Quick and efficient estimation procedures for the parameters which characterize physical decay in aerosol chamber trials,
 - (2) Aids useful in designing and interpreting chamber experiments
- (3) Procedures for testing the validity of the common assumptions with respect to physical decay, and

(4) Ways of evaluating the bias in methods of estimating biological recovery percentages which employ mass tracer data.

Finally and most important of all, these relationships constitute a start toward developing methods for testing the validity of the heterogeneous initial recovery model for biological recovery.

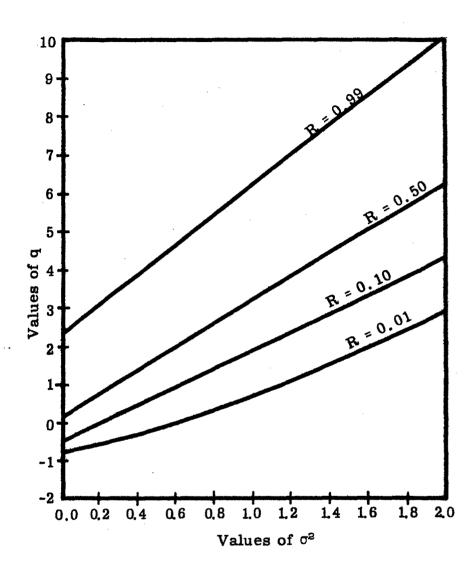


Figure 1. Graph of q versus $\sigma^{\text{\tiny 2}}$ for various values of R where

$$R = (1/\sqrt{2\pi}) \int_{-\infty}^{\infty} \exp\left[-1/2\right) v^2 - e^{-2(q-3\sigma^2 - v\sigma)} dv.$$

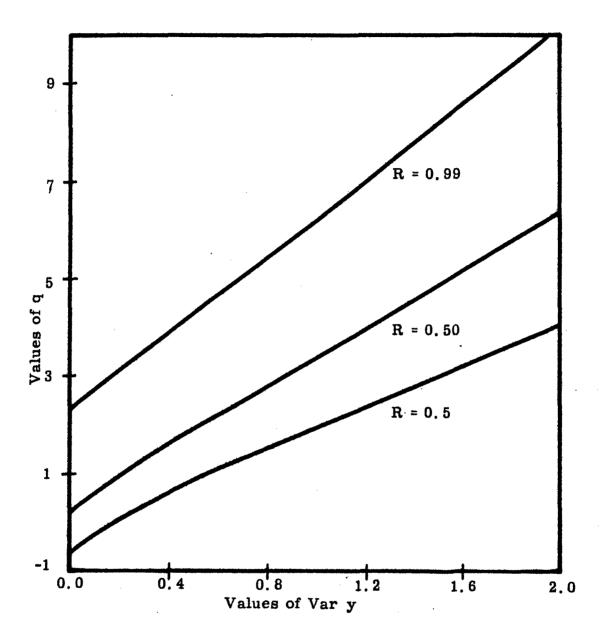


Figure 2. Values of q versus Var y at various physical recovery fractions.

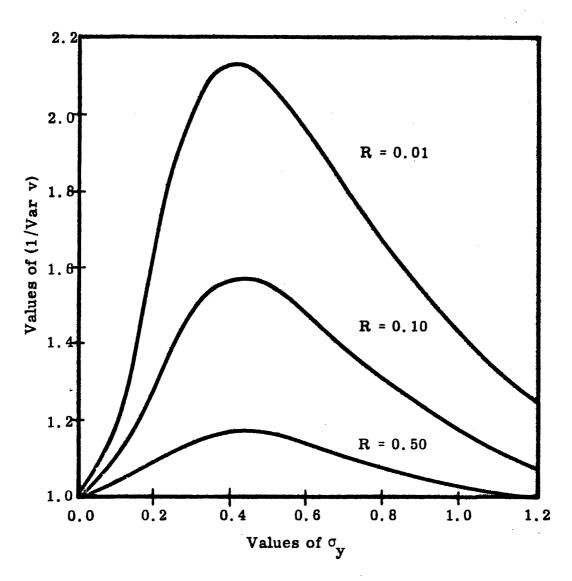


Figure 3. Values of (1/Var v) versus σ_y at various physical recovery fractions.

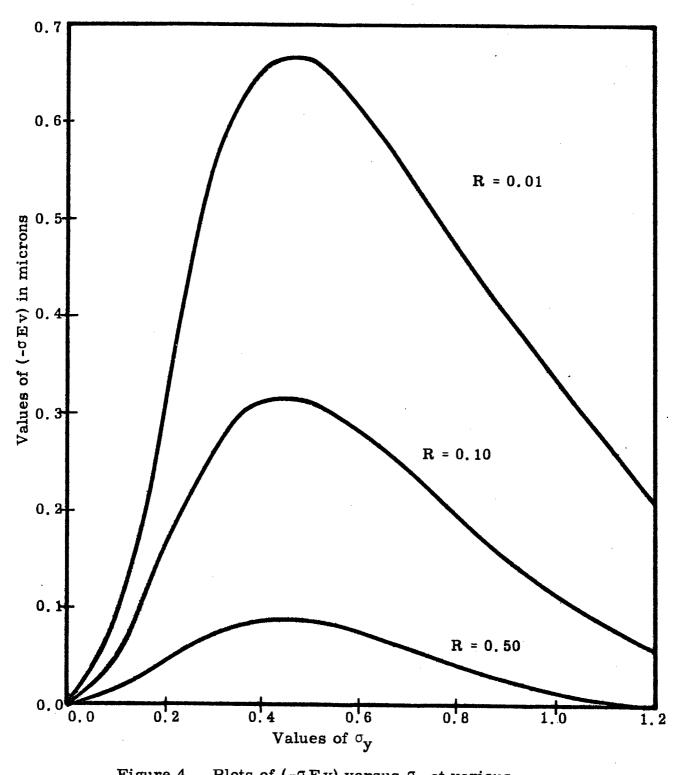


Figure 4. Plots of $(-\sigma E v)$ versus σ_y at various physical recovery fractions.